

# Cyclohexane, 1,2-dimethyl-, cis-

<b>Other names:</b>	1,2-Dimethylcyclohexane, cis 1,2-cis-Dimethylcyclohexane 1,2-cis-dimethylcyclohexane 1,CIS-2-DIMETHYLCYCLOHEXANE CIS-1,2-DIMETHYLCYCLOHEXANE Cyclohexane, 1,cis-2-dimethyl- c-1,2-Dimethylcyclohexane
<b>Inchi:</b>	InChI=1S/C8H16/c1-7-5-3-4-6-8(7)2/h7-8H,3-6H2,1-2H3/t7-,8+
<b>InchiKey:</b>	KVZJLSYJROEPSQ-OCAPTIKFSA-N
<b>Formula:</b>	C8H16
<b>SMILES:</b>	CC1CCCCC1C
<b>Mol. weight [g/mol]:</b>	112.21
<b>CAS:</b>	2207-01-4

## Physical Properties

Property code	Value	Unit	Source
af	0.2360		KDB
ap	314.850	K	KDB
chl	-5222.00 ± 1.80	kJ/mol	NIST Webbook
gf	41.24	kJ/mol	KDB
hcg	5222.93	kJ/mol	KDB
hcn	4870.846	kJ/mol	KDB
hf	-172.30	kJ/mol	KDB
hfus	9.38	kJ/mol	Joback Method
hvap	39.71	kJ/mol	NIST Webbook
hvap	39.70 ± 0.10	kJ/mol	NIST Webbook
hvap	39.40	kJ/mol	NIST Webbook
hvap	39.74	kJ/mol	NIST Webbook
hvap	39.70	kJ/mol	NIST Webbook
ie	10.08 ± 0.02	eV	NIST Webbook
ie	9.90 ± 0.07	eV	NIST Webbook
ie	9.78 ± 0.05	eV	NIST Webbook
log10ws	-4.30		Estimated Solubility Method
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	2940.00	kPa	KDB

rinpol	823.10	NIST Webbook
rinpol	834.10	NIST Webbook
rinpol	835.10	NIST Webbook
rinpol	839.10	NIST Webbook
rinpol	836.20	NIST Webbook
rinpol	829.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	831.00	NIST Webbook
rinpol	833.00	NIST Webbook
rinpol	836.00	NIST Webbook
rinpol	840.00	NIST Webbook
rinpol	830.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	850.00	NIST Webbook
rinpol	831.00	NIST Webbook
rinpol	836.00	NIST Webbook
rinpol	850.00	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	850.00	NIST Webbook
rinpol	826.60	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	827.20	NIST Webbook
rinpol	824.70	NIST Webbook
rinpol	824.40	NIST Webbook
rinpol	823.10	NIST Webbook
rinpol	824.70	NIST Webbook
rinpol	827.30	NIST Webbook
rinpol	834.90	NIST Webbook
rinpol	825.00	NIST Webbook
rinpol	840.20	NIST Webbook
rinpol	824.70	NIST Webbook
rinpol	827.30	NIST Webbook
rinpol	824.70	NIST Webbook
rinpol	834.70	NIST Webbook
rinpol	818.20	NIST Webbook
rinpol	822.00	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	836.00	NIST Webbook
rinpol	844.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	835.00	NIST Webbook
rinpol	827.00	NIST Webbook
rinpol	823.00	NIST Webbook

rinpol	829.00		NIST Webbook
rinpol	829.90		NIST Webbook
rinpol	832.50		NIST Webbook
rinpol	836.30		NIST Webbook
rinpol	839.10		NIST Webbook
rinpol	841.50		NIST Webbook
rinpol	843.50		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	824.40		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	829.10		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	827.10		NIST Webbook
rinpol	826.60		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	828.40		NIST Webbook
rinpol	828.40		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	828.80		NIST Webbook
rinpol	822.20		NIST Webbook
rinpol	826.70		NIST Webbook
rinpol	827.10		NIST Webbook
rinpol	826.90		NIST Webbook
rinpol	826.80		NIST Webbook
rinpol	826.60		NIST Webbook
rinpol	843.90		NIST Webbook
rinpol	832.40		NIST Webbook
rinpol	837.60		NIST Webbook
sg	374.34	J/molxK	NIST Webbook
tb	403.19 ± 0.50	K	NIST Webbook
tb	402.99 ± 0.30	K	NIST Webbook
tb	399.70 ± 2.00	K	NIST Webbook
tb	400.80 ± 3.00	K	NIST Webbook
tb	402.90	K	KDB

tb	402.90	K	NIST Webbook
tb	402.90	K	NIST Webbook
tb	403.00 ± 2.00	K	NIST Webbook
tb	403.00 ± 2.00	K	NIST Webbook
tb	403.19 ± 0.50	K	NIST Webbook
tb	403.00 ± 2.00	K	NIST Webbook
tb	402.70 ± 0.30	K	NIST Webbook
tb	402.88 ± 0.15	K	NIST Webbook
tb	402.87 ± 0.20	K	NIST Webbook
tb	394.00 ± 8.00	K	NIST Webbook
tb	402.70 ± 2.00	K	NIST Webbook
tb	402.70 ± 2.00	K	NIST Webbook
tb	402.15 ± 0.40	K	NIST Webbook
tb	402.85 ± 0.50	K	NIST Webbook
tb	402.99 ± 0.25	K	NIST Webbook
tb	402.80 ± 0.15	K	NIST Webbook
tb	402.99 ± 0.30	K	NIST Webbook
tb	403.40 ± 0.50	K	NIST Webbook
tb	402.87 ± 0.01	K	NIST Webbook
tb	403.25 ± 0.30	K	NIST Webbook
tb	401.15 ± 1.00	K	NIST Webbook
tb	398.00 ± 8.00	K	NIST Webbook
tb	403.33 ± 0.20	K	NIST Webbook
tc	606.00	K	KDB
tc	606.00	K	NIST Webbook
tf	222.97 ± 0.50	K	NIST Webbook
tf	222.97 ± 0.20	K	NIST Webbook
tf	222.93 ± 0.01	K	NIST Webbook
tf	223.10	K	KDB
tf	223.15 ± 0.07	K	NIST Webbook
tf	213.35 ± 0.50	K	NIST Webbook
tf	222.95 ± 0.30	K	NIST Webbook
tt	223.28 ± 0.01	K	NIST Webbook
tt	223.27 ± 0.05	K	NIST Webbook
vc	0.471	m <sup>3</sup> /kmol	KDB
zc	0.2750020		KDB

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.84	J/mol×K	530.89	Joback Method

cpg	247.23	J/molxK	464.10	Joback Method
cpg	230.28	J/molxK	430.71	Joback Method
cpg	212.54	J/molxK	397.32	Joback Method
cpg	293.52	J/molxK	564.28	Joback Method
cpg	307.47	J/molxK	597.67	Joback Method
cpg	263.41	J/molxK	497.49	Joback Method
dvisc	0.0018154	Paxs	218.77	Joback Method
dvisc	0.0009932	Paxs	254.48	Joback Method
dvisc	0.0006303	Paxs	290.19	Joback Method
dvisc	0.0004419	Paxs	325.90	Joback Method
dvisc	0.0003324	Paxs	361.61	Joback Method
dvisc	0.0041986	Paxs	183.06	Joback Method
dvisc	0.0002631	Paxs	397.32	Joback Method
hfust	1.64	kJ/mol	223.30	NIST Webbook
hvapt	33.47	kJ/mol	402.90	NIST Webbook
hvapt	33.64	kJ/mol	402.90	KDB
hvapt	34.50 ± 0.10	kJ/mol	387.00	NIST Webbook
hvapt	35.50 ± 0.10	kJ/mol	370.00	NIST Webbook
hvapt	38.00	kJ/mol	363.50	NIST Webbook
rfi	1.43358		298.15	KDB
rhol	796.00	kg/m3	293.00	KDB
srf	0.03	N/m	293.20	KDB

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37858e+01
Coeff. B	-3.21239e+03
Coeff. C	-5.25890e+01
Temperature range (K), min.	290.58
Temperature range (K), max.	431.66

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.35050e+01
Coeff. B	-7.12649e+03
Coeff. C	-8.66492e+00

Coeff. D	4.76986e-06
Temperature range (K), min.	223.16
Temperature range (K), max.	606.15

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Infinite dilution activity coefficients, specific retention volumes and NIST Webbook</b>	<a href="https://www.doi.org/10.1016/j.fluid.2006.07.015">https://www.doi.org/10.1016/j.fluid.2006.07.015</a>
<b>Estimation of thermodynamics of hydrocarbons in C7H158 branched alkane solvent.</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2207014&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2207014&amp;Units=SI</a>
<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a>
<b>Liquid Liquid Equilibria at Three Temperatures (between 280.15 K and 309.64 K) of Binary, Ternary, and Quaternary Systems Involving Methylcyclohexane, Water, Cyclohexane, para-Xylene, trans- and cis-Dimethylcyclohexane, and trans- and cis-Decahydronaphthalene:</b>	<a href="https://www.doi.org/10.1021/je500625r">https://www.doi.org/10.1021/je500625r</a> <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Solubilities of Alkylcyclohexanes in Water from 30 C to 180 C: The Yaws Handbook of Vapor Pressure: Apparatus for the Determination of Water Solubility in Hydrocarbon: Toluene and Alkylcyclohexanes (C6 to C8) from 30 C to 180 C:</b>	<a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=497">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=497</a> <a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=497">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=497</a> <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a> <a href="https://www.doi.org/10.1021/je0342567">https://www.doi.org/10.1021/je0342567</a> <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> <a href="https://www.doi.org/10.1021/je0502041">https://www.doi.org/10.1021/je0502041</a>

## Legend

<b>af:</b>	Acentric Factor
<b>ap:</b>	Aniline Point
<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hcg:</b>	Heat of Combustion, Gross form
<b>hcn:</b>	Heat of Combustion, Net Form
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rfi:</b>	Refractive Index
<b>rhoL:</b>	Liquid Density
<b>rinpol:</b>	Non-polar retention indices
<b>sg:</b>	Molar entropy at standard conditions
<b>srf:</b>	Surface Tension
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume
<b>zc:</b>	Critical Compressibility

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